

```

1  #-*- coding: utf-8 -*-
2  """
3  Created on Thu Mar 28 15:38:36 2019
4
5  @author: Nate
6  """
7
8
9  import numpy as np
10 import matplotlib.pyplot as plt
11 import pdb
12
13 '''
14 Use the Killingbeck method as presented in class to solve for the eigenvalues of the
15 hydrogen atom as in 1), but with greater accuracy. Use the same Verlet algorithm
16 to integrate backward to the origin from  $r = 25-50$ . Do Newton's iterations 4-10
17 times to find the correct  $e$  so that  $u(0,e) = 0$ . Determine the lowest energy levels of
18  $l = 0, 1, 2, 3$ . Use  $e = -0.6$  as your initial guess energy. Plot all energy values as a
19 function of  $dr$  from 0.01 to 0.1.
20 '''
21
22 delta_r = []
23 l_orbital = [0,1,2,3]
24 #l_orbital = [0]
25 energy_guess = -.6
26
27 #-1/r potential energies
28 for i in range(1,11):
29     #for i in range(1,50):
30     delta_r.append(i*.01)
31
32 #u(r+dr), u(r), l, r, energy_guess
33 def stepping(u_r_plus_dr, u_r, l, r, eps):
34     #fun = 2*(r*r/2) + l*(l+1)/r**2 - 2*eps
35     #pdb.set_trace()
36     fun = -2/r + l*(l+1)/r**2 - 2*eps
37     u_r_minus_dr = 2*u_r - u_r_plus_dr + delt_r**2*fun*u_r
38     return(u_r_minus_dr)
39
40 def stepping_for_v(v_r_plus_dr, v_r, u_r, l, r, eps):
41     #fun = 2*(r*r/2) + l*(l+1)/r**2 - 2*eps
42     #pdb.set_trace()
43     fun = -2/r + l*(l+1)/r**2 - 2*eps
44     v_r_minus_dr = 2*v_r - v_r_plus_dr + delt_r**2*fun*v_r + delt_r**2*-2*u_r
45     return(v_r_minus_dr)
46
47
48 #####
49 #####
50
51
52 good_points = []
53 to_plot = []
54
55
56 for l in l_orbital:
57     to_plot_holder = []
58     for delt_r in delta_r:
59
60         r = 100 - delt_r*2
61
62         for it in range(20): #8
63             u = [0, .01] #u_r_plus_dr, u_r
64             v = [0, .01]
65             #print(int(round(r/delt_r)))
66
67

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68         for i in range(int(round(r/delt_r))):
69             ...
70             u[0],u[1] = u[1], stepping(u[-2],u[-1], l, r, energy_guess)
71             v[0],v[1] = v[1], stepping_for_v(v[-2],v[-1], u[0], l, r, energy_guess)
72             #u.append(stepping(u[-2],u[-1], l, r, energy_guess))
73             ...
74             if u[0]*u[1] < 0:
75                 good_points.append([l, energy_guess, r])
76             ...
77             r-=delt_r
78             #u = [u[-2],u[-1]]
79             energy_guess = energy_guess - u[0]/(v[0]+.000001)
80             ...
81             #print("delta_r is: ", delt_r, " Energy is: ",energy_guess)
82             to_plot_holder.append([delt_r, energy_guess])
83             to_plot.append(to_plot_holder)
84             ...
85             #####
86             #####
87             #Plotting
88             ...
89             ...
90             ...
91             l0 = []
92             l1 = []
93             l2 = []
94             l3 = []
95             ...
96             for i in range(len(good_points)):
97                 if good_points[i][0] == 0:
98                     l0.append([good_points[i][1],good_points[i][2]])
99                 elif good_points[i][0] == 1:
100                     l1.append([good_points[i][1],good_points[i][2]])
101                 elif good_points[i][0] == 2:
102                     l2.append([good_points[i][1],good_points[i][2]])
103                 elif good_points[i][0] == 3:
104                     l3.append([good_points[i][1],good_points[i][2]])
105             ...
106             ...
107             fig1, axes1 = plt.subplots()
108             ...
109             axes1.scatter([to_plot[0][i][0] for i in range(len(to_plot[0]))], [to_plot[0][i][1] for
i in range(len(to_plot[0]))])
110             axes1.scatter([to_plot[1][i][0] for i in range(len(to_plot[1]))], [to_plot[1][i][1] for
i in range(len(to_plot[1]))])
111             axes1.scatter([to_plot[2][i][0] for i in range(len(to_plot[2]))], [to_plot[2][i][1] for
i in range(len(to_plot[2]))])
112             axes1.scatter([to_plot[3][i][0] for i in range(len(to_plot[3]))], [to_plot[3][i][1] for
i in range(len(to_plot[3]))])
113             axes1.set_ylabel('Energy')
114             axes1.set_xlabel('$\Delta r$')
115             axes1.set_title("Energy as a Function of $\Delta r$", va='bottom')
116             axes1.legend(['l=0', 'l=1', 'l=2', 'l=3'], loc='upper right')
117             plt.show()

```